Highlights: **Advanced Mathematical Methods for Electronic Structures, SciDAC SAP**

George Fann and Robert Harrison (ORNL)

We've developed the first massively parallel implementation of a multiresolution analysis solver with initial results on the ORNL Cray XT3. These initial results indicate excellent scalability up to 4096 processors. This demonstrates the outstanding scalability of this type of algorithms on terascale and the future petascale machines. We call our software Multiresolution Adaptive Numerical Evaluation for Scientific Simulation (MADNESS).

Capable of multiresolution analyses in multiwavelet bases, MADNESS serves as a powerful scientific framework for a number of important chemical problems. Potential applications include clean energy innovations for automobiles and industry (catalysis, fuel cells, combustion), improvements to the efficiency of drug development in the pharmaceutical field, and analysis of the dynamics of molecules and electrons in powerful new laser fields. The MADNESS software provides several levels at which applications can be programmed. A high-level single-instruction multiple-data (SIMD) environment is suitable for rapid application development. An asynchronous variant of the single-program multiple-data (SPMD) environment provides more scalability at the price of increased programmer awareness of data flow. Finally, a multiple-instruction multiple data (MIMD) environment is suitable for the development of new, high-performance kernels on petascale computing platforms.

The scalability of the fundamental operations is plotted below.